Automatic Mass Spectral Deconvolution and Identification Software (AMDIS)

The problems of establishing chemical identity for trace species in complex matrices breaks down into two distinct pieces – isolating a single species and then analyzing the species so isolated. The tool of choice for many such complex matrices is the gas chromatograph coupled to the mass spectrometer. The data needed for identification of the species by mass spectrometry and NIST's role in providing it is discussed in Reference Libraries of Mass Spectra. The problem addressed here is the isolation of the individual species.

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The nature of the chromatographic process is that it is never complete, and thus there are often multiple components coming out "together" so that the mass spectral signatures are not clean enough to allow identification. The need is to determine what ions that are present belong to one component *vs.* another. The disentanglement is called deconvolution and is accomplished by a software expert system termed ***"Automatic Mass Spectral Deconvolution and Identification Software"*** (AMDIS) using a series of algorithms developed at NIST with funding from the Defense Department in order to aid in the compliance with the Chemical Weapons Convention. The broader utility of the tool for analysis of complex mixtures (such as surface waters for pollutants, food for contamination, complex fluids for medical applications) is only now being realized.

The fundamental algorithms that make up AMDIS are very stable. Only the most modest changes have been needed. However, in response to needs by the chemical instrumentation industry, AMDIS has evolved to handle new instruments, to better couple to instrumentation software and to deal with types of analyses for which it was not originally designed. As a result, we have worked very closely with a number of instrumentation companies to assist the development of tools to make the use of AMDIS by their customers easier. In addition, we have been working directly with laboratories that are developing tools to respond to possible terrorism events where very large numbers of samples will need to be analyzed at possibly very sensitive levels.

Perhaps the most important accomplishment this year was the incorporation of AMDIS into a product distributed by Agilent Technologies to aid their users with AMDIS. The utility of AMDIS had been recognized by Agilent, but it had not been easy to get their customers to use AMDIS due to the perceived difficulty of the software. Agilent built a tool to allow their users to work more closely with the software they are accustomed to (the Agilent instrument software) and use that to access AMDIS. The result, a product that Agilent distributes called Deconvolution Reporting Software (DRS), has allowed a broader range of chemists to make use of the power of AMDIS. In addition, Agilent coupled the output of AMDIS to further analysis with the NIST MS Search software to allow the users a high degree of confidence in the final result.

Agilent Technologies

The release of AMDIS 2.64 (AMDIS Download Page) occurred in December of 2005.

For the most part, the release was a maintenance release to fix a number of small bugs that had been noted. One important major change was the addition of a new help file and manual. The previous version of these had fallen behind the program and so a major revision of both the help file and manual were done.

There have been a number of minor changes in direct response to user input. The most important has been to provide the user with better values for the area of the component and allow the user to specify a single ion to be used to calculate areas for concentration calculations. This has been the most widely requested addition to AMDIS. The area calculations were compared to the values using software currently used on some specific instruments and the agreement was found to be quite good. This latter is especially important since there is a wide acceptance of the methodology of the instrument-specific calculation. Additional changes made in response to user requests are a method of using only specific ions (and not the total ion current (TIC)) for analysis and improvements in the ability of the program to use results from searching the NIST database.

AMDIS provides the first broadly available method for automating GC/MS analysis. It offers a tool for finding, with high confidence, components in complex mixtures that would otherwise be impossible to identify.

AMDIS can significantly increase the productivity of analysts in the laboratory by doing the first pass analysis in minutes – without direct intervention, rather than hours – with full involvement of the analyst. AMDIS can also aid in providing statistically valid confidence measures for analysis.

The use of AMDIS is steadily increasing; it is widely used as part of the proficiency exams for laboratories world wide to demonstrate compliance with the Chemical Weapons Convention. Increasingly it is being used for metabolite studies in complex matrices such as whole plant and whole cell analysis. Finally, the adoption of AMDIS as a part of the new DRS system of Agilent has increased the number of users of the NIST product.

Future Plans:

The development of AMDIS will continue to be driven by the user community. Specific plans include minor modifications in the algorithm to take into account varying scan ranges as are often used in the instrumentation, and improved access to the algorithm using the DLL (dynamic link library) in order to facilitate the use by instrument companies within their own data systems.

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Publications and Presentations

- Mallard, W.G., ***"Chemical Analysis and the Chemical Weapons Convention – On-Site Analysis, Databases, OPCW Designated,"*** American Society for Mass Spectrometry (ASMS) Sanibel Conference: Mass Spectrometry in Forensic Science & Counterterrorism, Clearwater Beach, FL, January 29, 2005.
- Mallard, W.G., ***"AMDIS and Chemical Identification – Development Tools For Use With Food Emergency Response Laboratories",*** Forensic Chemistry Center, U.S. Food & Drug Administration, Cincinnati, OH, February 15, 2005
- Mallard, W.G., ***"Rates of False Positive Identification using Selected Ion Analysis"***, Air Lab Conference, Midwest Research Institute, Melrose, FL, February 24, 2005
- Mallard, W.G., ***"AMDIS and Chemical Identification – Analysis Tools for Pesticide Residues"***, NIST Presentations at PittCon, Orlando, FL, March 2, 2005
- Mallard, W.G., ***"AMDIS and Chemical Identification – Analysis Tools for Pesticide Residues"***, Chemical Residue Laboratory, Florida Department of Agriculture and Consumer Services, Tallahassee, FL, April 6, 2005
- Mallard, W.G., ***"AMDIS and Portable MS"***, Inficon Corp, Syracuse, NY, July 26, 2005
- Mallard, W.G., ***"AMDIS and Chemical Identification – Introduction to the Software"***, Agilent Technologies, Beijing, China, August 16, 2005.
- Mallard, W.G., ***"Extending AMDIS – Interactions with Instrument Software, Concentration Calculations and Increased Sensitivity"***, Agilent Technologies, Wilmington, DE, November 17, 2005.